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14. ABSTRACT
This collaborative project aims at the study of the global resolution of convex programs with complementarity constraints (CPCCs), which form a large subclass of the class of mathematical programs with complementarity constraints MPCCs). Despite the large literature on the local properties of an MPCC, there is a lack of systematic investigation on the computation of a globally optimal solution of these constrained optimization problems, or in the case where such a solution does not exist, on the generation of a certificate demonstrating the solution non-existence. While this is by no means an easy task, the pervasiveness of the CPCC in applications provides an important motivation for the undertaking of this project. As a first step in our study, we have focused on the class of linear programs with linear complementarity constraints (LPCCs), which is essentially a linear program with additional complementarity constraints on certain pairs of variables. Subsequently, we have extended our work to the class of convex quadratic programs with complementarity constraints (QPCCs). Much research remains to be done; we believe that our work so far has provided a solid foundation for the global resolution of this highly challenging class of practically important constrained optimization problems.

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Final Report

Collaborative AFOSR grants FA9550-08-1-0081 and FA9550-08-1-0061

Project Period: from March 01, 2008 to November 30, 2010

Project Title: Global Resolution of Convex Programs with Complementarity Constraints

Principal Investigators: John E. Mitchell (Rensselaer Polytechnic Institute) and Jong-Shi Pang (University of Illinois at Urbana-Champaign)

This collaborative project aims at the study of the global resolution of convex programs with complementarity constraints (CPCCs), which form a large subclass of the class of mathematical programs with complementarity constraints (MPCCs). Despite the large literature on the local properties of an MPCC, there is a lack of systematic investigation on the computation of a globally optimal solution of these constrained optimization problems, or in the case where such a solution does not exist, on the generation of a certificate demonstrating the solution non-existence. While this is by no means an easy task, the pervasiveness of the CPCC in applications provides an important motivation for the undertaking of this project. As a first step in our study, we have focused on the class of linear programs with linear complementarity constraints (LPCCs), which is essentially a linear program with additional complementarity constraints on certain pairs of variables. Subsequently, we have extended our work to the class of convex quadratic programs with complementarity constraints (QPCCs). Much research remains to be done; we believe that our work so far has provided a solid foundation for the global resolution of this highly challenging class of practically important constrained optimization problems.

Publications: The publications that resulted from these grants are summarized as follows.

• J. Hu, J.E. Mitchell, and J.S. Pang. An LPCC approach to nonconvex quadratic programs. *Mathematical Programming* (2011) in print.

Abstract. Filling a gap in nonconvex quadratic programming, this paper shows that the global resolution of a feasible quadratic program (QP), which is not known a priori to be bounded or unbounded below, can be accomplished in finite time by solving two linear programs with linear complementarity constraints, i.e., LPCCs. Specifically, this task can be divided into two LPCCs: the first confirms whether the QP is bounded below on the feasible set and, if not, computes a feasible ray on which the QP is unbounded; the second LPCC computes a globally optimal solution if it exists, by identifying a stationary point that yields the best quadratic objective value. In turn, the global resolution of these LPCCs can be accomplished by a parameter-free, mixed integer-programming based, finitely terminating algorithm developed recently by the authors, which can be enhanced in this context by a

new kind of valid cut derived from the second-order conditions of the QP and by exploiting the special structure of the LPCCs. Throughout, our treatment makes no boundedness assumption of the QP; this is a significant departure from much of the existing literature which consistently employs the boundedness of the feasible set as a blanket assumption. The general theory is illustrated by 3 classes of indefinite problems: QPs with simple upper and lower bounds (existence of optimal solutions is guaranteed); same QPs with an additional inequality constraint (extending the case of simple bound constraints); and nonnegatively constrained copositive QPs (no guarantee of the existence of an optimal solution). We also present numerical results to support the special cuts obtained due to the QP connection. Online at `http://www.rpi.edu/~mitchj/papers/QP_unbdd.html`

• J. Hu, J.E. Mitchell, J.S. Pang, and B. Hu. On linear programs with linear complementarity constraints. *Journal of Global Optimization* (2011) in print.

Abstract. The paper is a manifestation of the fundamental importance of the linear program with linear complementarity constraints (LPCC) in disjunctive and hierarchical programming as well as in some novel paradigms of mathematical programming. In addition to providing a unified framework for bilevel and inverse linear optimization, nonconvex piecewise linear programming, indefinite quadratic programs, quantile minimization, and L_0 minimization, the LPCC provides a gateway to a mathematical program with equilibrium constraints, which itself is an important class of constrained optimization problems that has broad applications. We describe several approaches for the global resolution of the LPCC, including a logical Benders approach that can be applied to problems that may be infeasible or unbounded. Online at `http://www.rpi.edu/~mitchj/papers/LPECmodels.html`

• J.S. Pang. Three modeling paradigms in mathematical programming. *Mathematical Programming, Series B*, 125 (2010) 297–323.

Abstract. Celebrating the sixtieth anniversary since the zeroth International Symposium on Mathematical Programming was held in 1949, this paper discusses several promising paradigms in mathematical programming that have gained momentum in recent years but have yet to reach the main stream of the field. These are: competition, dynamics, and hierarchy. The discussion emphasizes the interplay between these paradigms and their connections with existing subfields including disjunctive, equilibrium, and nonlinear programming, and variational inequalities. We will describe the modeling approaches, mathematical formulations, and recent results of these paradigms, and sketch some open mathematical and computational challenges arising from the resulting optimization and equilibrium problems. Our goal is to elucidate the need for a systematic study of these problems and to inspire new research in the field.

• J.E. Mitchell, J.S. Pang, and B. Yu. Obtaining tighter relaxations of mathematical programs with complementarity constraints. *Proceedings of MOPTA 2010, Modelling and Optimization: Theory and Applications*, submitted (February 2011).

Abstract. The class of mathematical programs with complementarity constraints (MPCCs)

constitutes a powerful modeling paradigm. In an effort to find a global optimum, it is often useful to examine the relaxation obtained by omitting the complementarity constraints. We discuss various methods to tighten the relaxation by exploiting complementarity, with the aim of constructing better approximations to the convex hull of the set of feasible solutions to the MPCC, and hence better lower bounds on the optimal value of the MPCC. Better lower bounds can be useful in branching schemes to find a globally optimal solution. Different types of linear constraints are introduced, convex quadratic constraints are constructed, and semidefinite programming constraints are also discussed. These constraints are typically applicable to any convex program with complementarity constraints. Computational results for linear programs with complementarity constraints (LPCCs) are included, comparing the benefit of the various constraints on the value of the relaxation, and showing that the constraints can dramatically speed up the solution of the LPCC. Online at `http://www.rpi.edu/~mitchj/papers/tightenGeneralCuts.html`

Manuscripts in Progress: In addition to the above completed work, two manuscripts are presently in their final stage of completion.

• J.E. Mitchell, J.S. Pang, and B. Yu. Convex quadratic relaxations of nonconvex quadratically constrained quadratic programs.

Abstract. Nonconvex quadratic constraints can be linearized to obtain relaxations in a well-understood manner. We propose to tighten the relaxation by using second-order cone constraints, resulting in a convex quadratic relaxation. Our quadratic approximation to the bilinear term is compared to the linear McCormick bounds. The second-order cone constraints are based on linear combinations of pairs of variables. With good bounds on these combinations, the resulting constraints are stronger than the McCormick bounds. Computational results are given.

• L. Bai, J.E. Mitchell, and J.S. Pang. On convex quadratic programs with complementarity constraints.

Abstract. The present paper shows that the global resolution of a general convex quadratic program with complementarity constraints (QPCC), not known in advance to be feasible or solvable, can be accomplished in finite time. To accomplish this, a minmax mixed integer formulation is set up by introducing finitely many binary variables, one for each complementarity constraint. Based on the primal-dual relationship of a pair of convex quadratic programs, an extreme ray/point generation logical Benders scheme is developed, which relies on valid inequalities for the integer program expressed in the form of satisfiability constraints. To make this scheme more efficient, we propose a two-stage approach wherein the first stage solves the mixed integer quadratic program (by an available solver) with an additional constraint that bounds the sum of the complementarity variables, and the second stage solves the program outside this bounded region by the Benders scheme. We report computational results with our method. We also investigate the addition of a penalty term $y^T Dw$ to the objective function, where y and w are complementary variables and D is a nonnegative diagonal matrix. The matrix D can be chosen efficiently by solving a semidefinite program, in

order to ensure that the objective function remains convex. For our test problems, the addition of the penalty term can often reduce the overall runtime by at least 50%. In addition, we report preliminary computational testing on a method based on the S-lemma which can be used to obtain better lower bounds from infeasible points, by obtaining bounds on their distance from infeasibility; this method could be incorporated into a branching scheme.

Research in Progress: The PIs continue to engage in interdisciplinary research wherein the MPCC paradigm provides a fundamental approach for solving applied hierarchical decision-making problems. Two ongoing projects are: (a) the solution of Stackleberg games with Nash-Cournot players arising from electricity markets and biofuel production and planning, and (b) the estimation of pure characteristics models in empirical marketing research. Both of these problems lead to QPCCs for which the methodology described above could be applied. While some progress has been made, inverse quadratic programs of realistic sizes, such as the bi-parameter identification problem in support-vector machines (SVM), remain elusive to be efficiently solved by the advances made so far. Exact solution to bi-parameter SVM models is one topic in Bin Yu's thesis, and we expect to complete a paper describing his results in the spring; these results are far better than those that could be obtained through a direct use of an integer programming solver such as CPLEX. These problems, and a new emergent model—the discretely-constrained MPCC, are some of the topics that the PIs are pursuing in their extended study that is being built on the results obtained from the AFOSR grants.

Student Supervision: The grants have provided partial support of several Ph.D. students in their thesis research. Jing Hu, who obtained her doctoral degree from Rensselaer Polytechnic Institute (RPI) in August 2009, was co-supervised by the two PIs. Two other students are presently supervised by PI Mitchell at RPI: Bin Yu will defend his Ph.D. thesis in Spring 2011 and Lijie Bai is presently in the second year of her Ph.D. work. Yuching Lee, who is presently in her third year, is supervised by PI Pang at the University of Illinois at Urbana-Champaign.

Doctoral Theses:

• **Jing Hu**: Graduated August 2009.

This thesis was the basis for the two papers "An LPCC approach to nonconvex quadratic programs" and "On linear programs with linear complementarity constraints". Another chapter of her thesis was incorporated into an earlier paper, "On the Global Solution of Linear Programs with Linear Complementarity Constraints", by J. Hu, J.E. Mitchell, J.S. Pang, K.P. Bennett, and G. Kunapuli, *SIAM Journal on Optimization* 19 (1) 2008, pages 445-471. She developed a logical Benders decomposition approach to globally solve LPCCs without the need to introduce a "big-M" parameter. Her taxonomy of classes of LPCCs will aid in the formulation and solution of additional problems with complementarity constraints. The global optimization approach for nonconvex quadratic programs is applicable even to problems with unbounded feasible regions; one of its strengths is the construction of cutting planes based on second order optimality conditions, which can dramatically tighten up the

LPCC formulation. Online at `http://www.rpi.edu/~mitchj/phdtheses/jing/rpithes.pdf`

Summary of Jing Hu's thesis:
A linear program with linear complementarity constraints plays the same important role in the studies of MPECs as a linear program does in convex programs in addition to many direct applications of its own. Since an LPCC is a special case of an MPEC, many existing computational methods for solving MPECs can be applied to solve LPCCs, including regularization and active set methods. Yet these methods have invariably focused on obtaining a stationary solution that is not guaranteed to be globally optimal for the LPCC. Particularly impressive among these methods are those state-of-art nonlinear programming based solvers which do not rely on the existence of an interior point, such as FILTER which has been used as a benchmark in our computational experiments. One method to globally resolve an LPCC is to introduce a large parameter "big-M", reformulate the LPCC as a mixed-integer problem, and apply various integer programming based techniques to the problem. The deficiency of such an approach is that it assumes the existence of this conceptual parameter "big-M"; in other words, this method is only applicable to the LPCCs that attain finite optimal solutions. A major contribution of this dissertation lies in the parameter-free integer-programming based cutting-plane algorithm presented in Chapter 3 for globally resolving a general LPCC; that is, our method is capable of determining the following three states of an LPCC with valid certificates: the LPCC is infeasible, the LPCC is feasible and unbounded, or the LPCC is optimally solvable. In addition, our algorithm is able to determine on which piece the objective is unbounded for the second case; or compute a global optimal solution of the LPCC for the last case.

The remainder of this dissertation is focused on indefinite quadratic programming, which forms an important application of the LPCCs. This is one of the most important subjects in mathematical programming, playing an essential role in nonlinear programming in addition to many of its own direct applications. There is now an extensive list of literature devoted to this subject; much of which is based on nonlinear programming techniques and the computed solutions are generally stationary points only. The algorithms developed for globally resolving QPs have invariably presumed its solvability, that is the QP is known in advance to attain a finite optimal solution. The research on the global resolution of indefinite QPs which are not known a priori to be bounded or unbounded on their feasible regions, still remains unresolved until now. It is well known that the QP with finite optima can be resolved by solving an equivalent LPCC reformulation. Inspired by this approach, we have proposed an LPCC approach that is able to identify the QPs which have unbounded objective values on the feasible regions. In this approach, an LPCC is formulated based on the given QP and the global resolution of this LPCC is able to provide a valid certificate of the unboundedness of the QP.

This dissertation consists of several fairly independent chapters. Chapter 2 provides a short review of numerous applications of LPCCs in science, engineering and finance. We have briefly described each application and defined the mathematical formulation for each problem. Although there still exist many other applications arising from different areas, we

hope that this short summary will at least give a basic idea of why LPCCs are receiving more attention in mathematical programming, and hope that these efforts can stimulate further research on this subject.

In Chapter 3, we have presented a parameter-free IP based algorithm (Section 3.4) for the global resolution of an LPCC and reported computational results (Section 3.5) obtained from the application of the algorithm for solving a set of randomly generated LPCCs of moderate sizes. The results show that our algorithm is able to successfully identify infeasible or unbounded LPCCs, and also compute the globally optimal solutions of the LPCCs if they exist. Continued research may be conducted on refining the algorithm. For instance, it is found from the experiments that much of the computational efforts were consumed on solving the LPs in the sparsification step. Thus a possible refinement is to find ways to sparsify a cut with more efficiency; in other words, can the sparsification step be implemented without solving too many LPs? Moreover, the algorithm can be applied to realistic classes of LPCCs, such as bilevel machine learning problems and many other practical problems described in Chapter 2. The detailed applications should be explored.

In Chapter 4, we have investigated an LPCC approach to the global resolution of indefinite, possibly unbounded quadratic programs. The main contributions of this research are as follows. First of all, we have introduced an LPCC whose global resolution will certify whether or not the QP attains finite optima (Theorem 13 and Corollary 14). Secondly, we have identified some valid inequalities for the MIP formulation of the LPCC which is an equivalent formulation of a solvable QP. These inequalities, which are motivated by the second-order optimality conditions of the QP (Proposition 16), are expected to improve the efficiency of the LPCC approach. Moreover we have described a new algorithm for solving box-constrained QPs (Subsection 4.4.1). Computational results have been shown to support the promise of the LPCC approach to indefinite QPs (Section 4.5). These are all positive contributions to the study of indefinite QPs. Yet this research is just the first step in developing a general algorithm for globally resolving non-convex QPs; in particular, further study is needed to understand better about the LPCC (4.9) and its MIP formulation, in order to derive deeper cuts and sharper LP relaxations in the sparsification of these cuts.

• **Bin Yu**: Expected to graduate May 2011.

As part of his thesis, Bin contributed to the two papers "Obtaining tighter relaxations of mathematical programs with complementarity constraints" and "Convex quadratic relaxations of nonconvex quadratically constrained quadratic programs." Further, we expect to publish at least two further papers based on his doctoral research. The first paper will be on a branch-and-cut approach to solving LPCCs. As part of this work, Bin developed a novel primal heuristic, investigated several different branching schemes, and incorporated various types of cutting planes; the resulting implementation is considerably faster than a CPLEX implementation using indicator constraints for most of our test instances. The second paper will be on the application of the branch-and-cut approach to the bi-parameter identification problem in support-vector machines. This is an important class of problems in data analysis with multiple applications. In the literature, these problems are attacked using heuristics, which provide no guarantee of global optimality. Our approach does result in a global op-

timum. We can solve instances with hundreds of observations that are intractable for a standard CPLEX implementation, although the largest instances we can solve is perhaps smaller than might be desired in real-world applications.

Presentations: The PIs and their students have presented the results of this research at various conferences and institutions as described below.

Jong-Shi Pang:

• 20th International Symposium on Mathematical Programming (Chicago; August 2009)

• International Conference on Linear Programming Algorithms and Extensions (Haikou, China; May 2009)

• Department of Computer and Systems Science "Antonio Ruberti" University of Rome "La Sapienza" (Rome; January 2009)

• Industrial Engineering and Management Sciences Department, Northwestern University (Evanston; November 2008)

• Industrial, Manufacturing & Systems Engineering Department, Hong Kong University (Hong Kong; October 2008)

• AFOSR Optimization and Discrete Mathematics Annual Review (Arlington, VA; April 2008)

John Mitchell:

• Industrial & Systems Engineering Department, Lehigh University (Bethlehem, PA; November 2010)

• MOPTA 2010 (Bethlehem, PA; August 2010)

• AFOSR Optimization and Discrete Mathematics Annual Review (Arlington, VA; April 2009 and 2010)

• Second Waterloo Engineering Optimization Day (Plenary talk; Waterloo, Ontario; March 2010)

• 20th International Symposium on Mathematical Programming (Chicago; August 2009)

• IMA Hot Topics Workshop: Mixed-Integer Nonlinear Optimization: Algorithmic Advances and Applications, (Minneapolis; November 2008)

• INFORMS (Washington DC; October 2008)

Jing Hu:

• INFORMS (Washington DC; October 2008)

Yu-Ching Lee:

- 20th International Symposium on Mathematical Programming (Chicago; August 2009)
- INFORMS poster session (Austin, Texas; November 2010)

Bin Yu:

- INFORMS (Austin, Texas; November 2010)
- INFORMS (San Diego; October 2009)
- 20th International Symposium on Mathematical Programming (Chicago; August 2009)